Finite Element Modeling of Crystal Deformations in Neutron Diffraction Experiments

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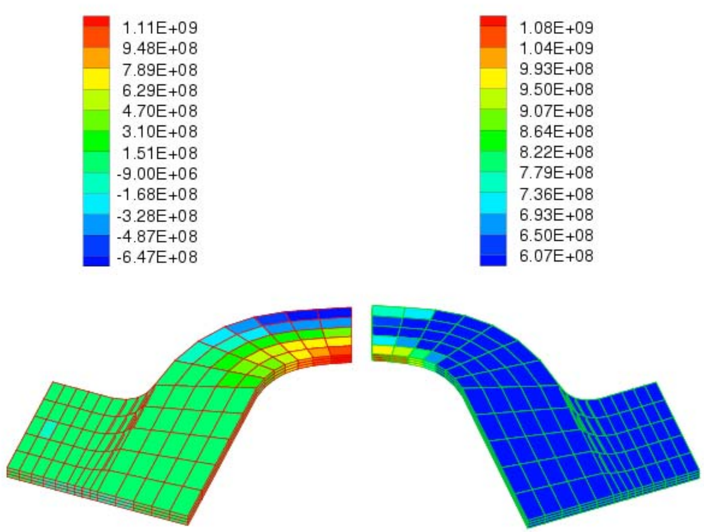

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Overview

Develop simulation models for metal plasticity:

- Large-strain elasto-plastic responses
- Polycrystalline, polyphase alloys
- Responses under monotonic and cyclic loadings

Obtain reliable predictions of:

- Structure/state evolution with deformation
- Stresses from intragrain to component scale

Difficulties:

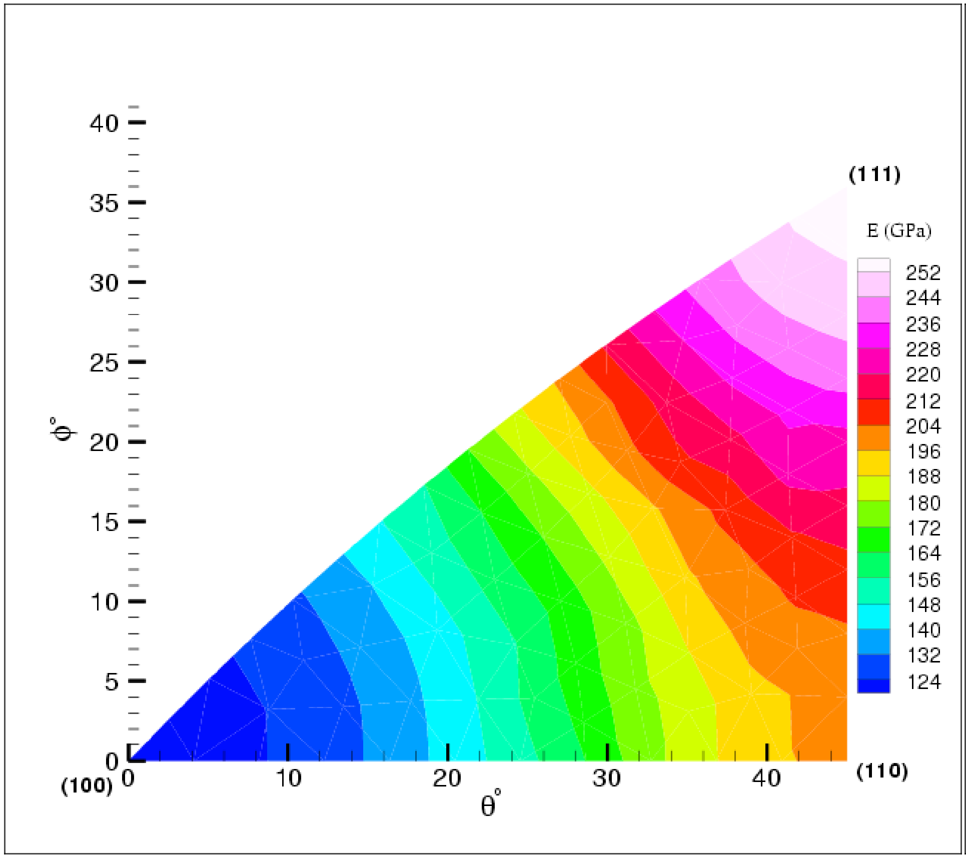
- Identifying of single crystal properties
- Initializing the state (texture, strength, lattice strains)
- Modeling grain (crystal) interactions
- Accounting for inherent structure variability (statistical distributions)

Approach:

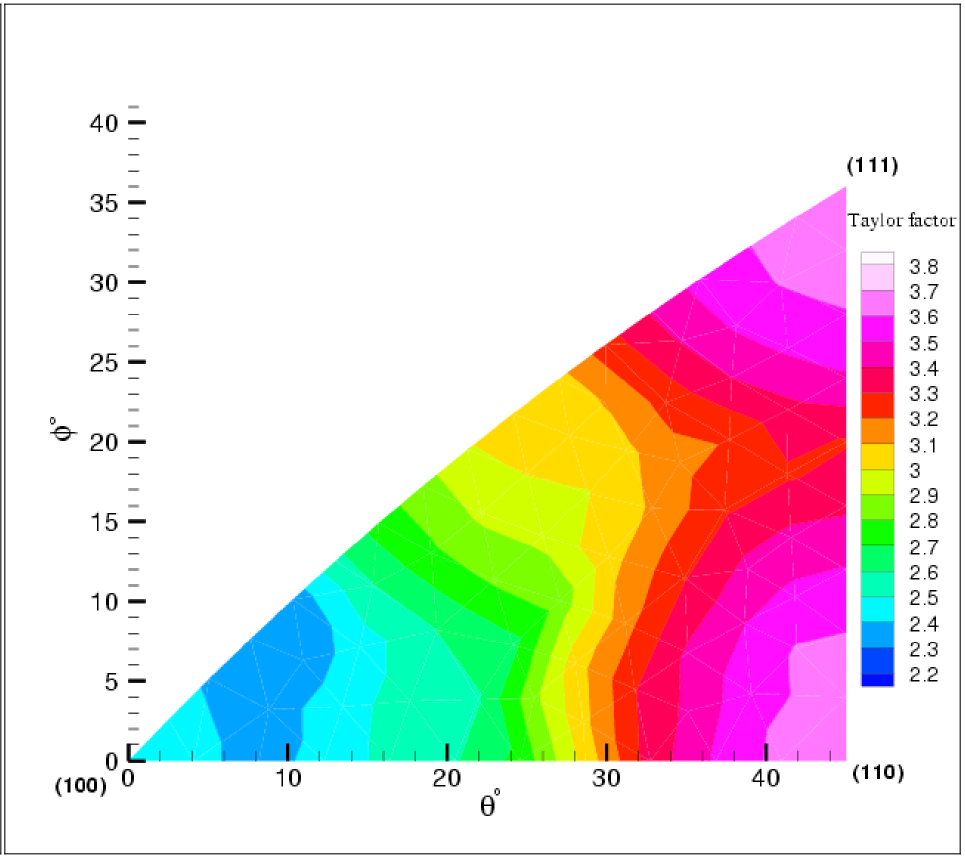
- Utilize an iterative **Build ➲ Compare ➲ Critique ➲ Modify** methodology
- Data for comparison are from diffraction experiments

Crystal Elastic and Plastic Properties

Directional Modulus (elastic)



Taylor Factor (plastic)



- Stiffness/strength orientation dependence
- Strong influence on grain interactions
- Suggests importance of *in situ* testing

Modeling Approach

Constitutive model:

- Anisotropic elasticity (cubic for FCC)
- Restricted slip (12 {111}<110> systems for FCC)
- Power law kinetics for slip (rate insensitive)
- Modified Voce hardening

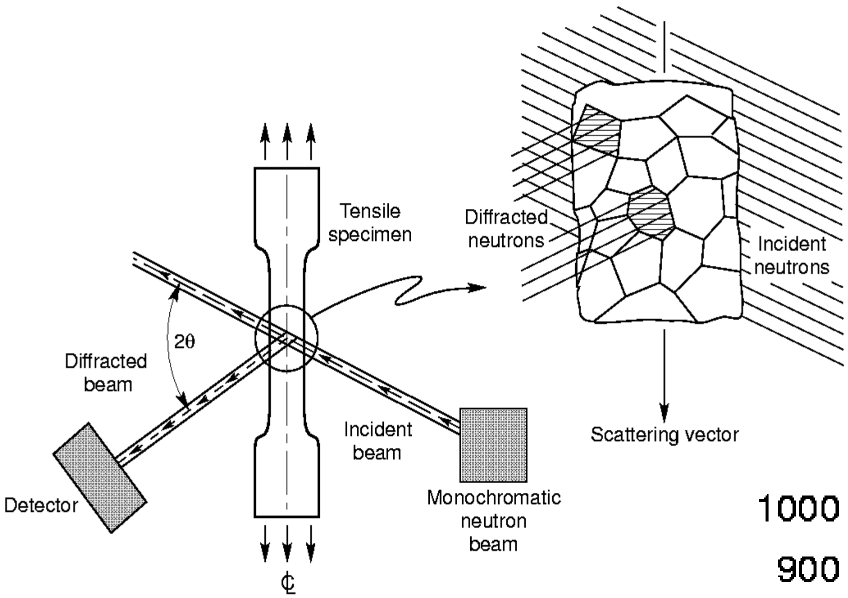
Finite element methodology:

- 3-D velocity-pressure formulation
- Residuals on equilibrium and mass conservation
- Geometric nonlinearity with updated Lagrangian reference

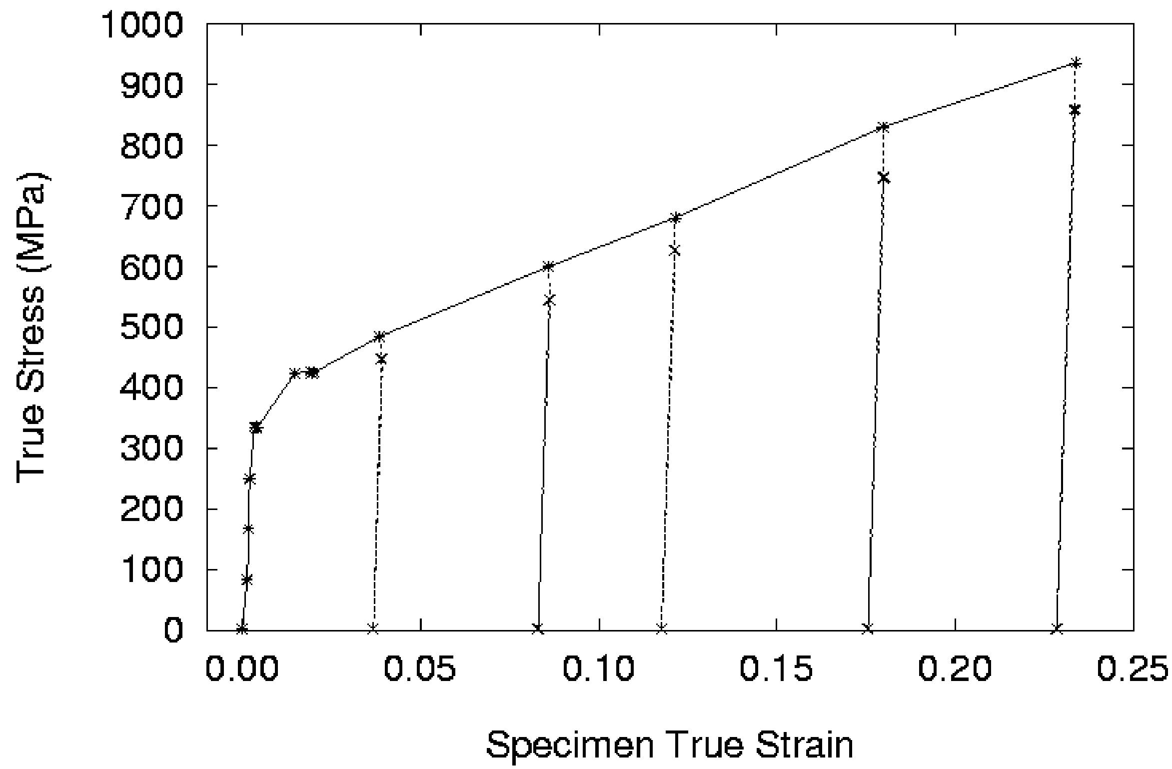
Computer implementation:

- Scalable parallel using MPI and F90
- Performed on IBM-SP or Intel Velocity Cluster

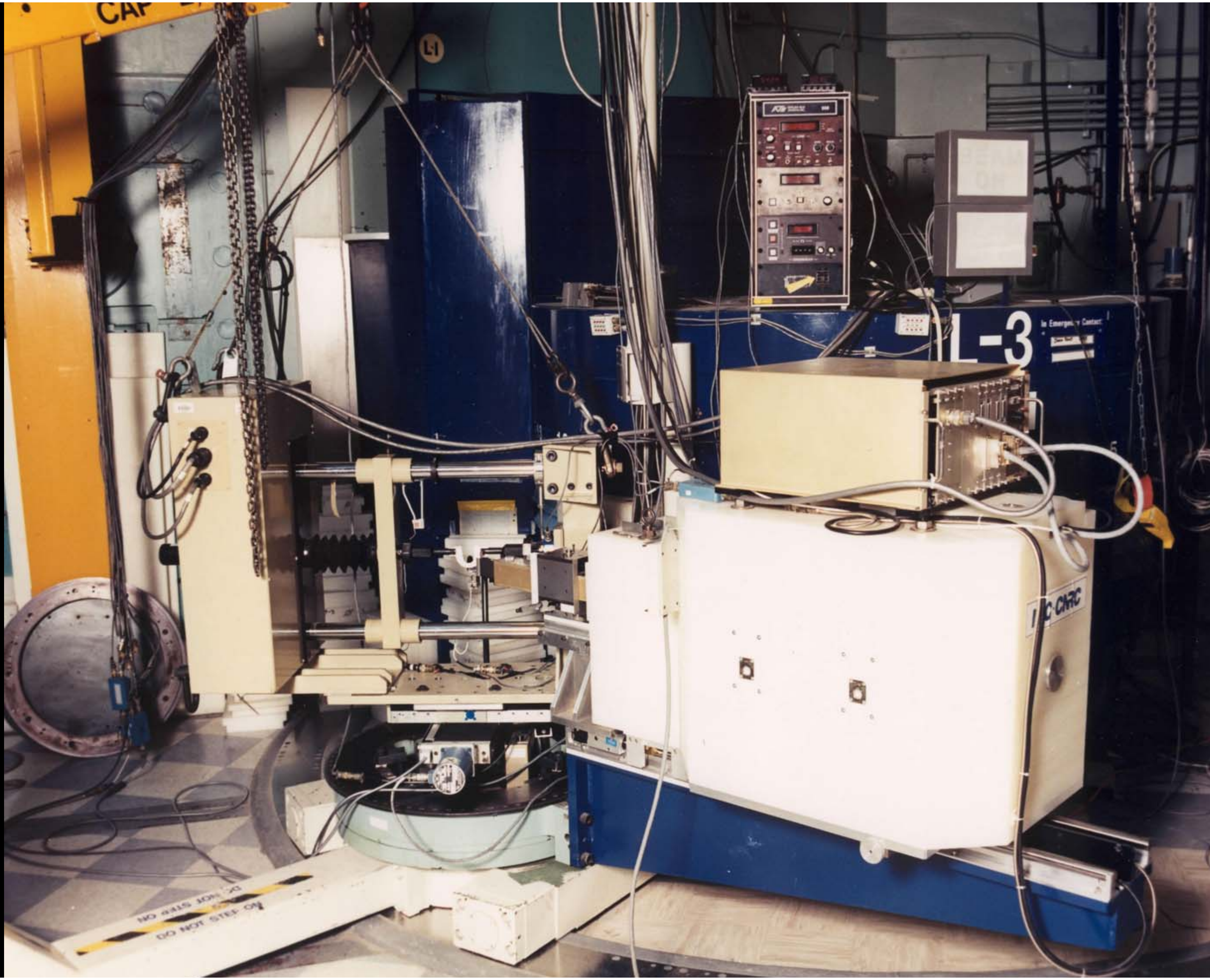
Neutron Diffraction Experiments



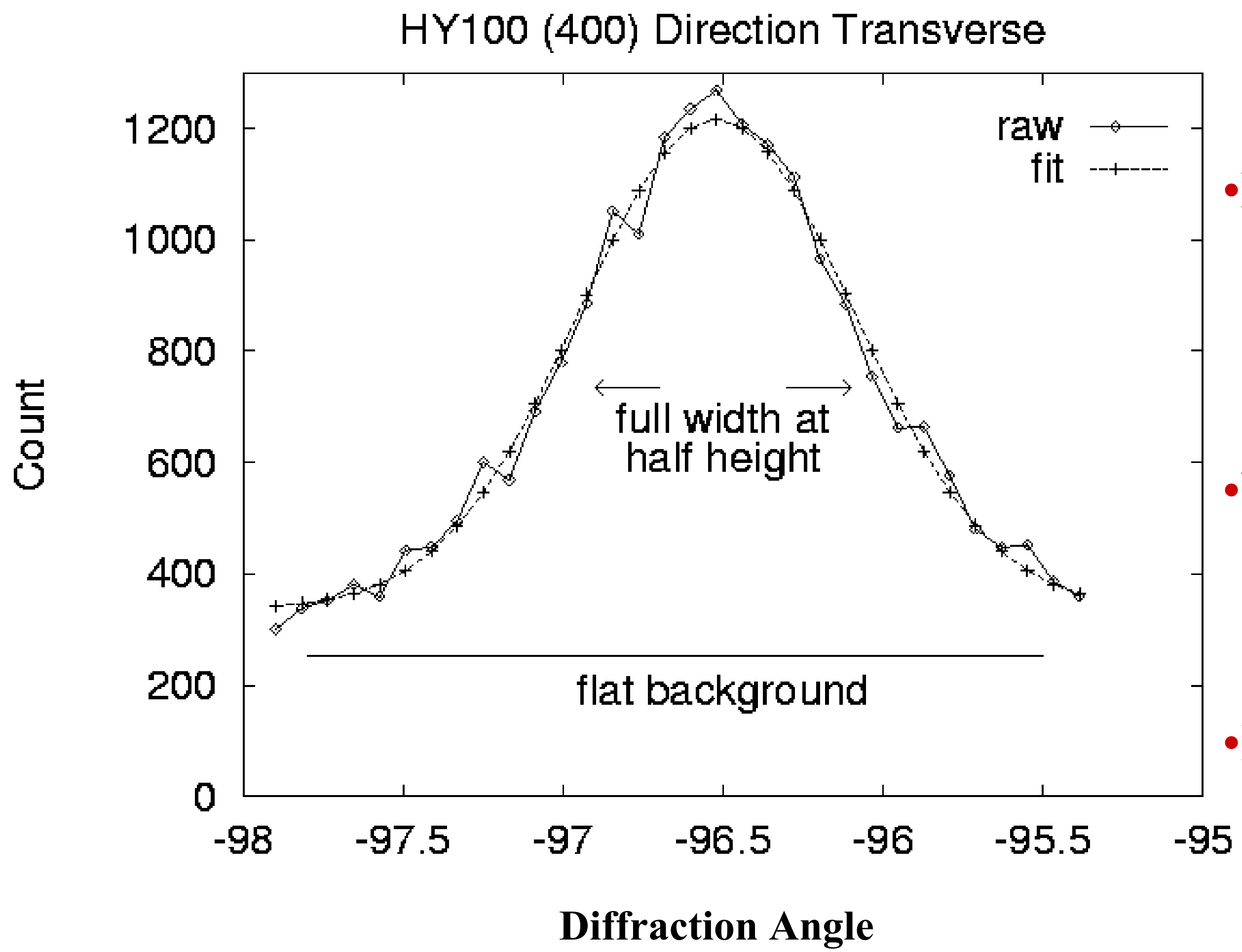
- (200), (220), (222) and (311) reflections
- Axial and transverse scattering vectors



- Five unloading episodes
- Diffraction measurements points labeled (x)


L-1
L-3
In Emergency Contact
DO NOT STEP ON
DO NOT STEP ON

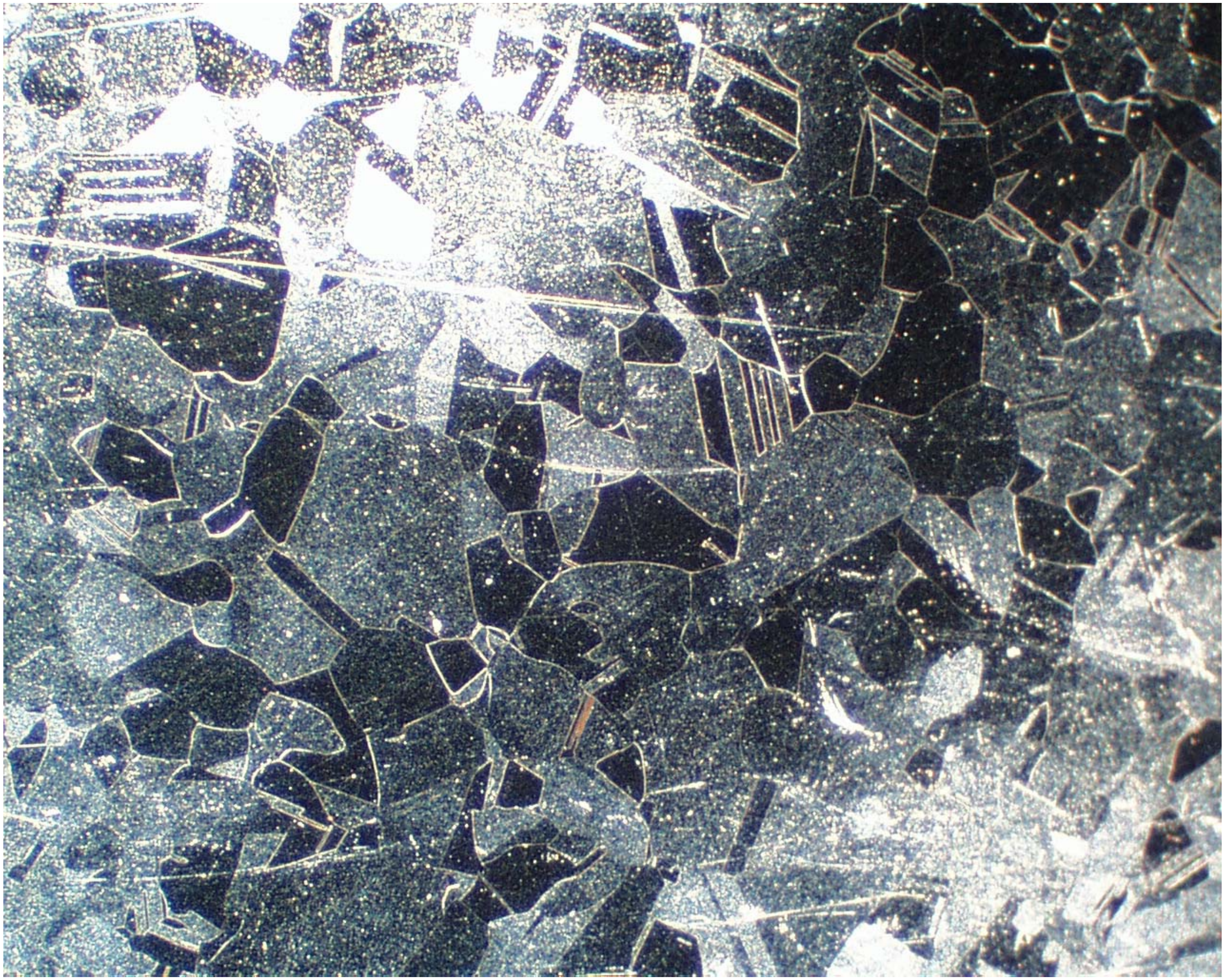
Diffraction Peak Data



- •Position → Average lattice strain
- •Width → Includes dislocation density
- •Intensity → Texture component strength

Examine the (400), (311), (222) and (220) lattice planes (peaks).

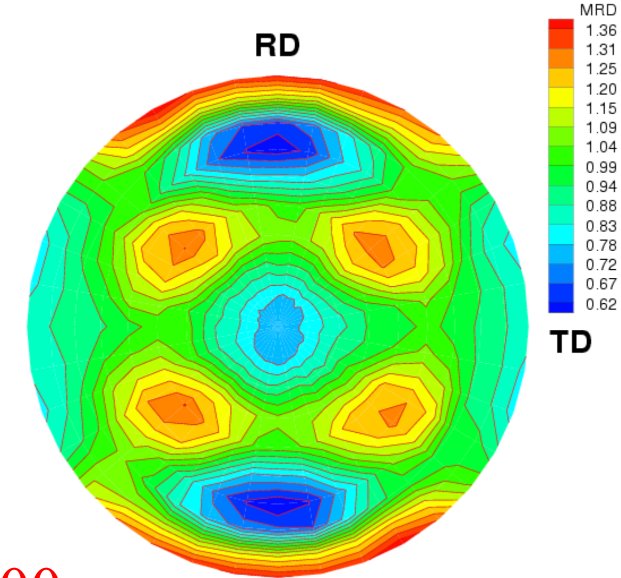
Micrograph at 200X of AL6XN Sample



Etchant selected to highlight grain boundaries

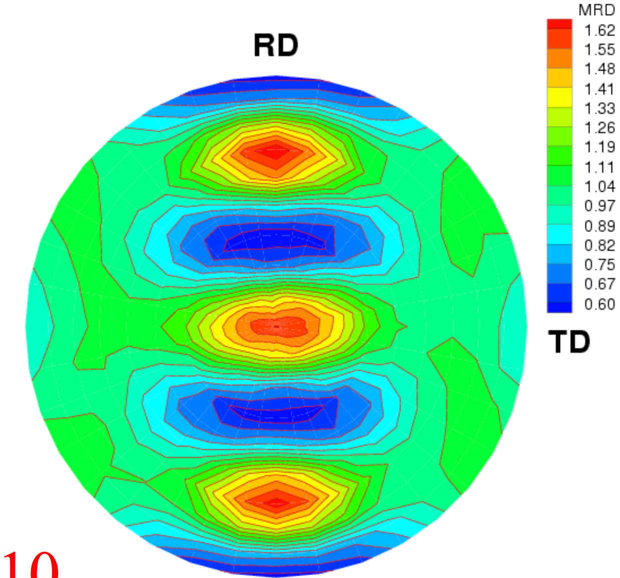
50 µm

AL 6XN Pole Figures



100

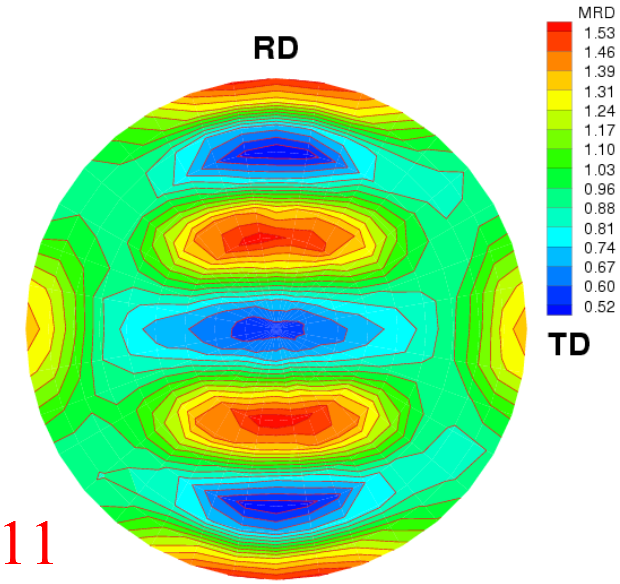
100 Pole Figure
Bulk - Neutron Diffraction
15 degree averaging radius



110

110 Pole Figure
Bulk - Neutron Diffraction
15 degree averaging radius

- Measured by neutron diffraction
- Rolling texture
- Used to evaluate ODF

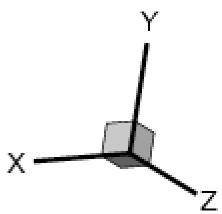


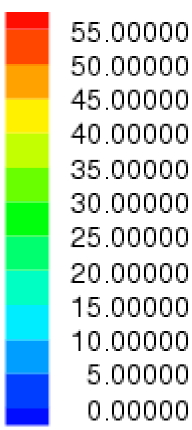
111

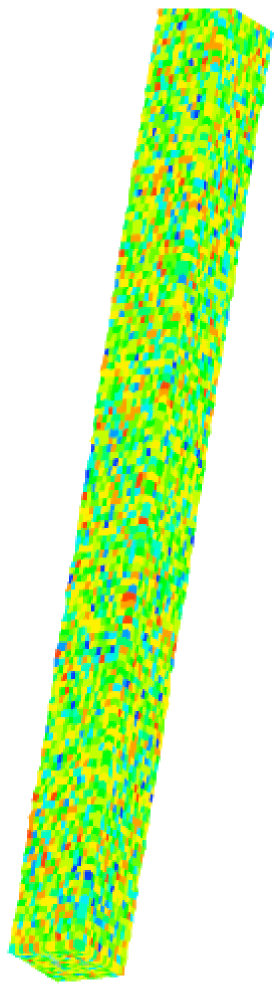
111 Pole Figure
Bulk - Neutron Diffraction
15 degree averaging radius

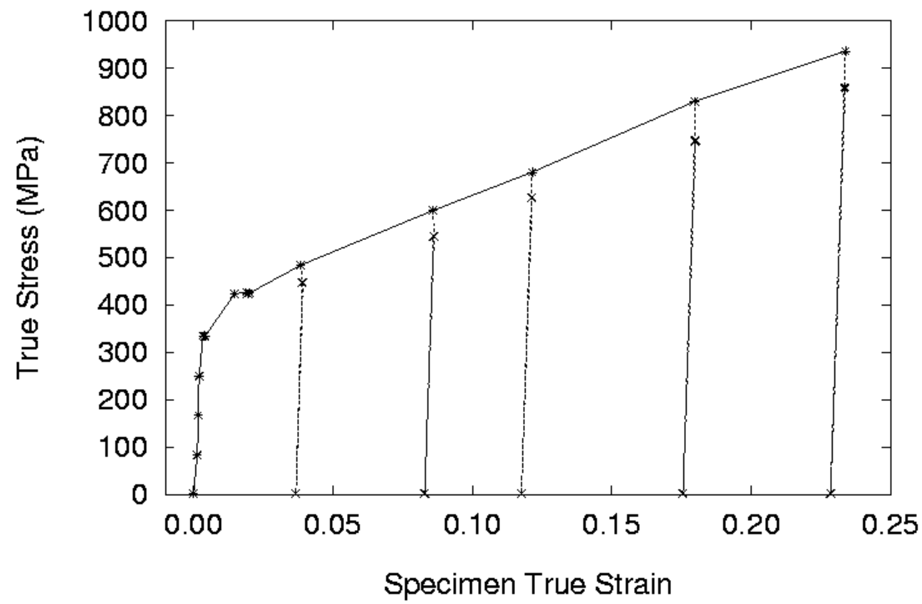
Crystal-Scale Finite Element Simulation

Angle between crystal (100) and sample [010] directions







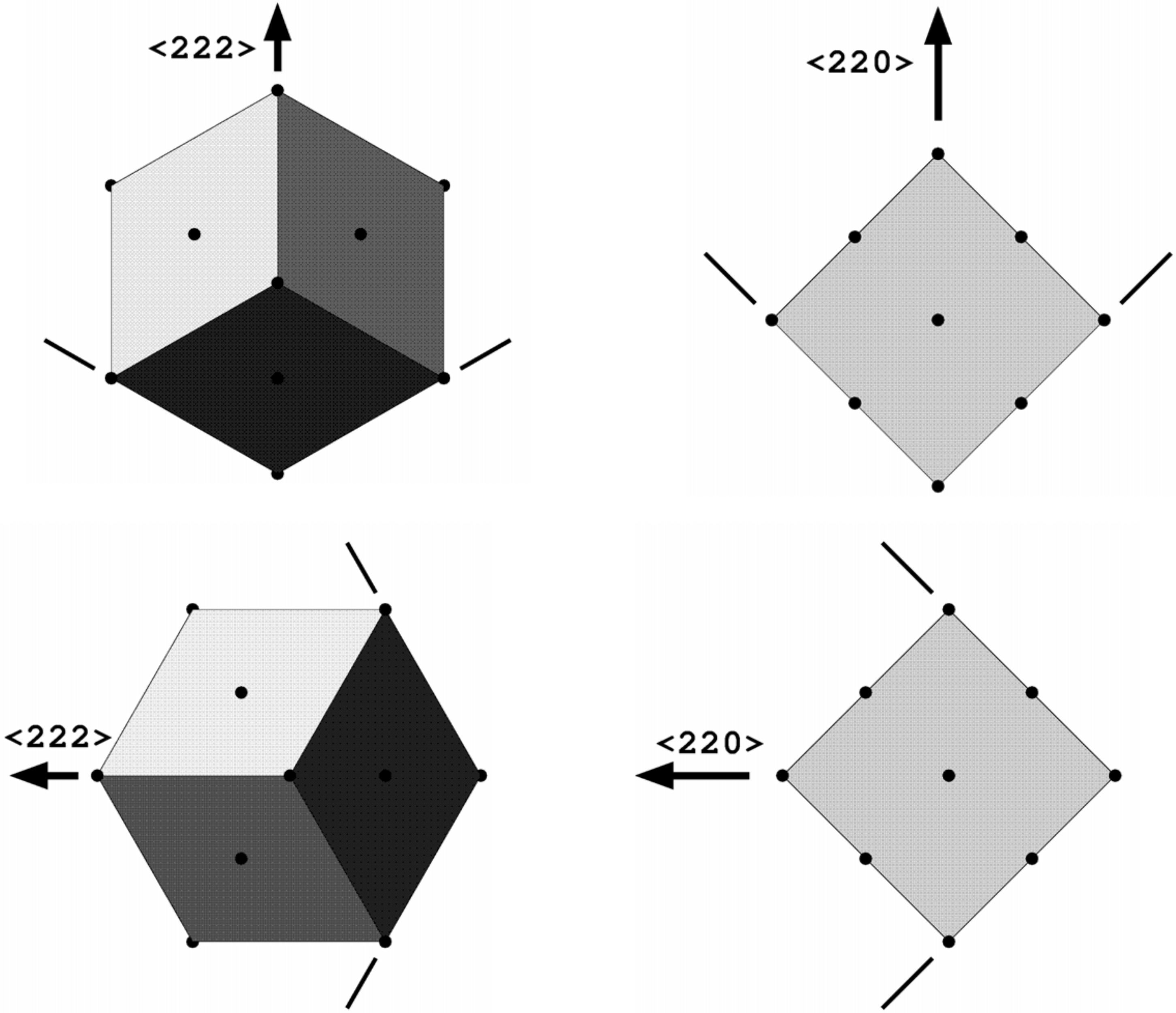


- Tensile loading along Y axis
- 28,800 finite elements
- Orientation after deformation
- Initial orientation from measured texture

Scattering Vectors and Crystal Planes

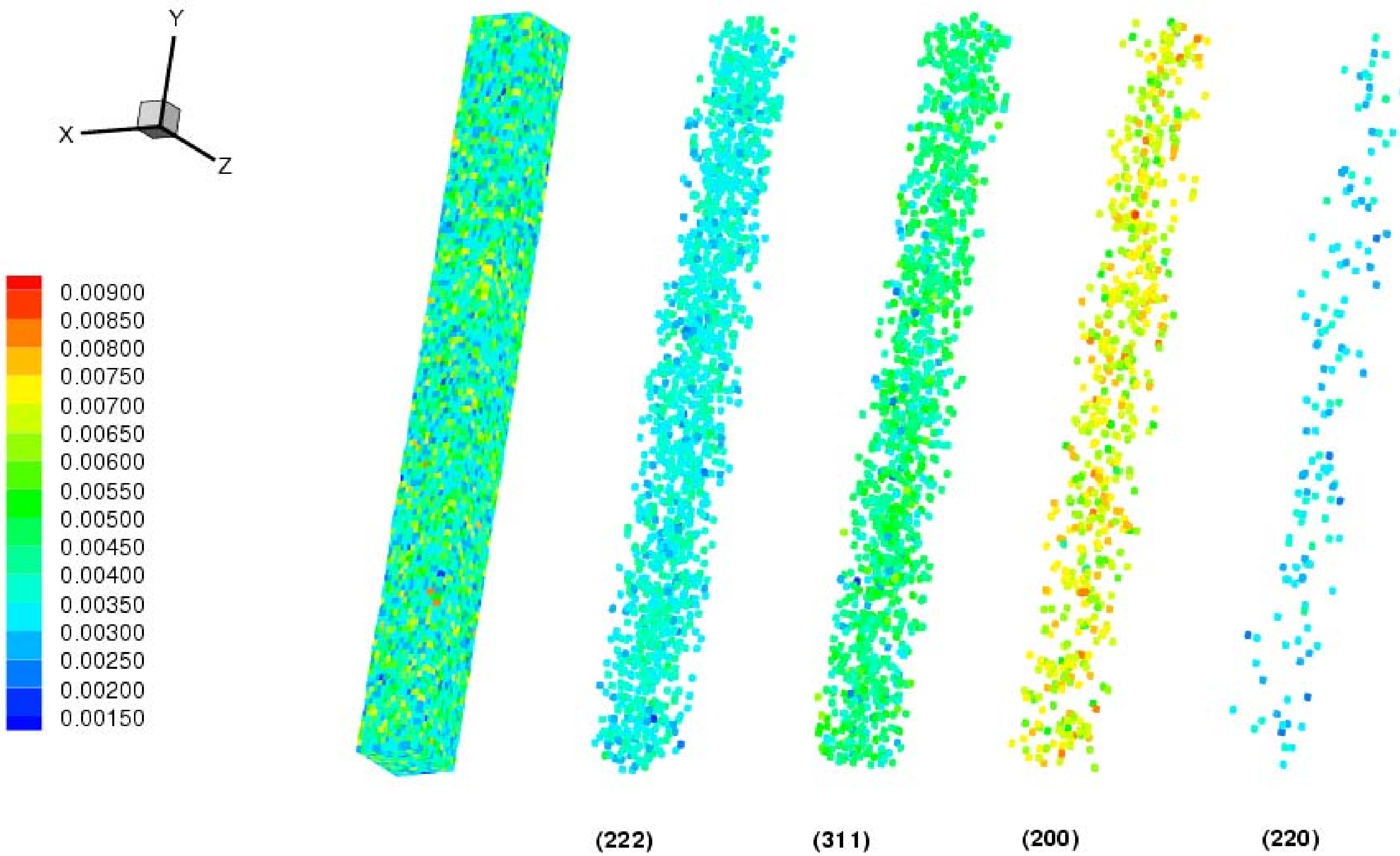
Axial scattering vectors

Lateral scattering vectors



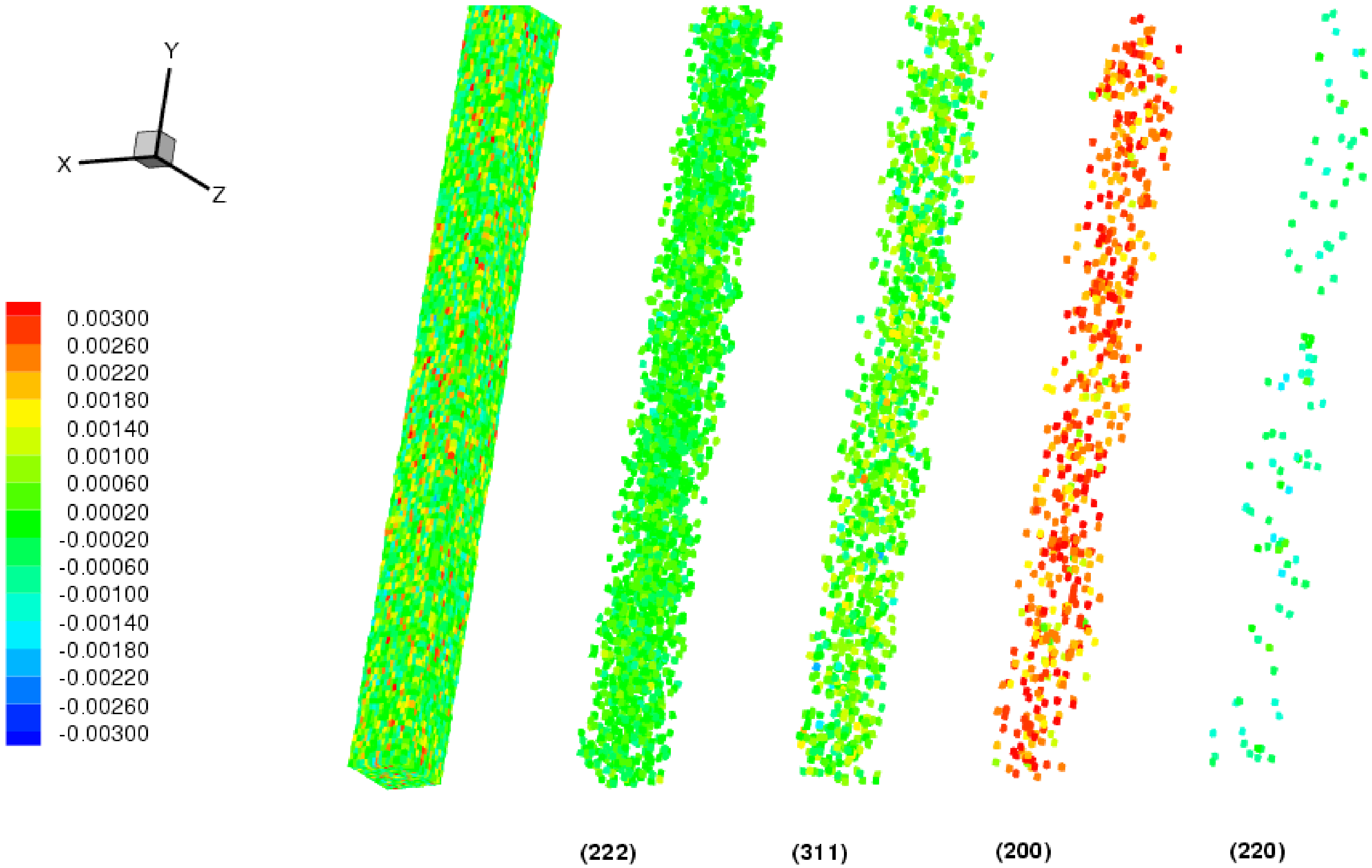
Lattice Strains at Final Loading

- Axial scattering vector
- Plate TD direction
- Specimen/Plate: x/RD; y/TD; z/ND

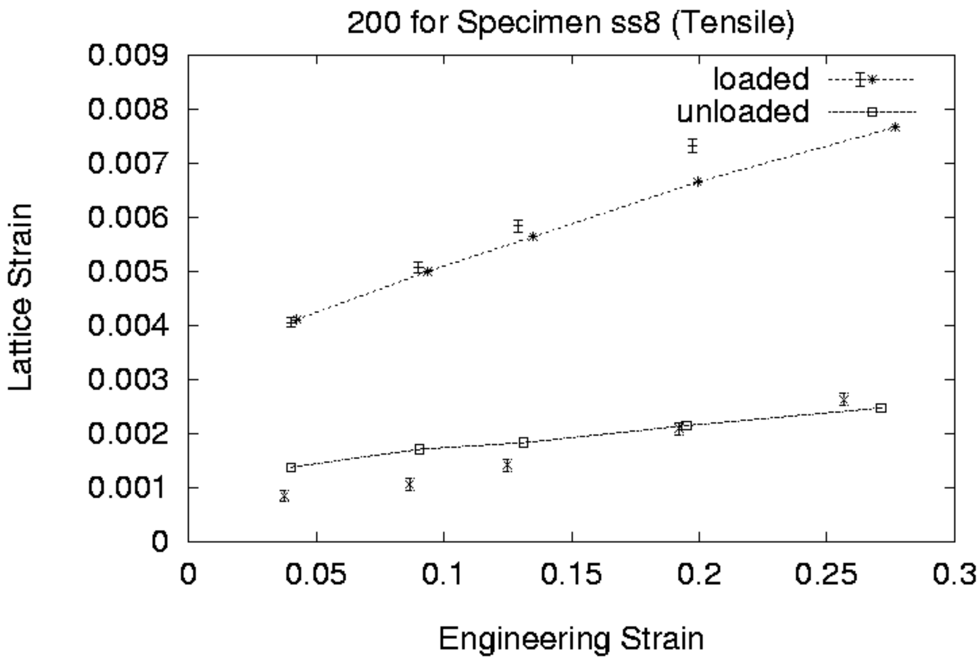


Lattice Strains at Final Unloading

- Axial scattering vector
- Plate TD direction
- Specimen/Plate: x/RD; y/TD; z/ND



(200) Crystals

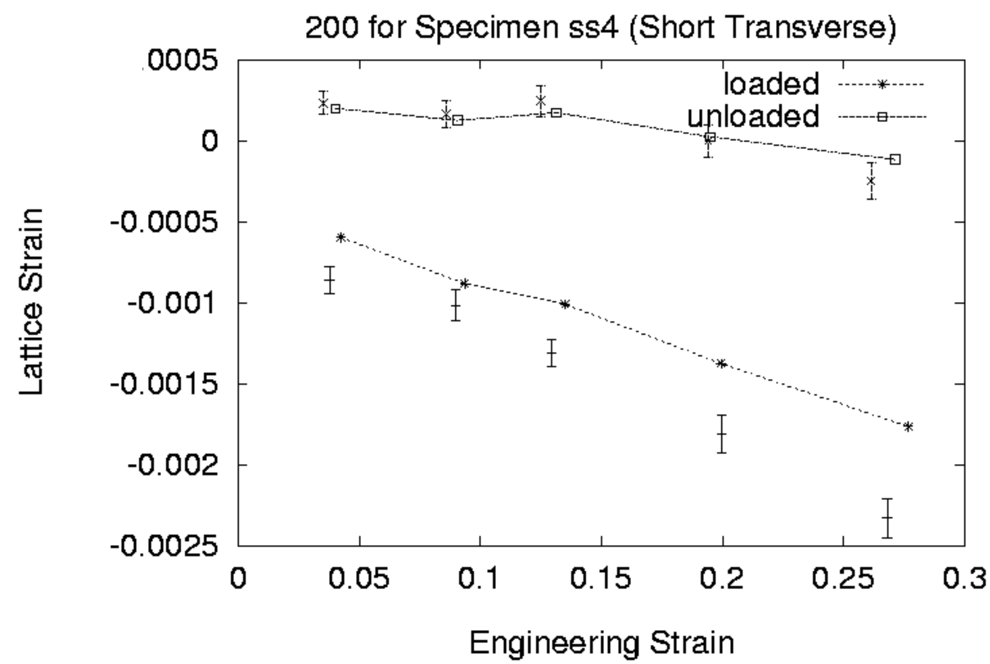


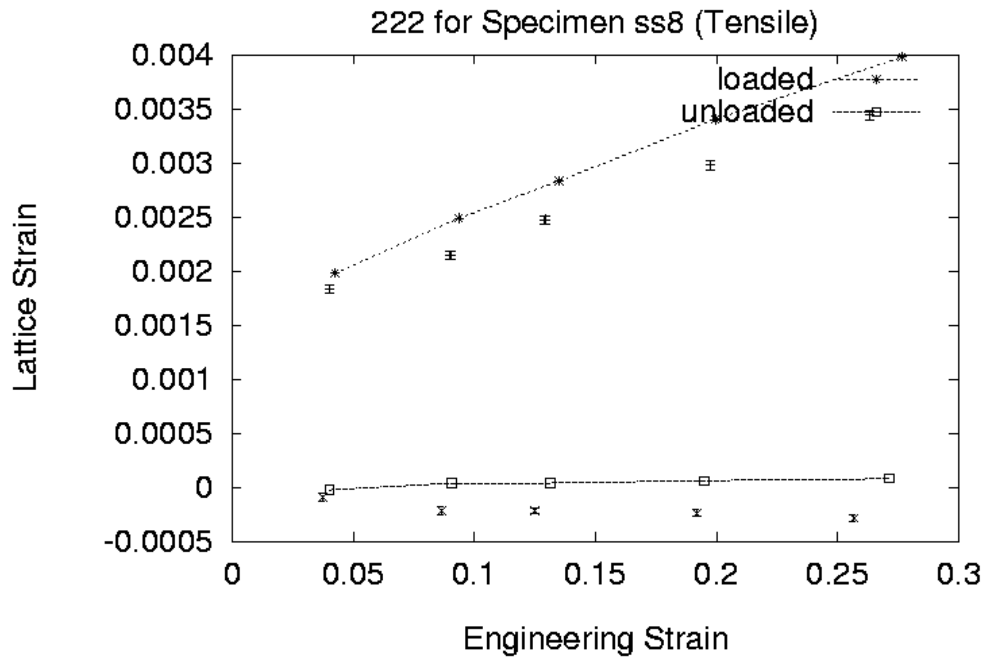
Axial Lattice Strains

- Upper curves - loaded
- Lower curves - unloaded
- Data points with error bars

Lateral Lattice Strains

- Lower curves - loaded
- Upper curves - unloaded
- Data points with error bars





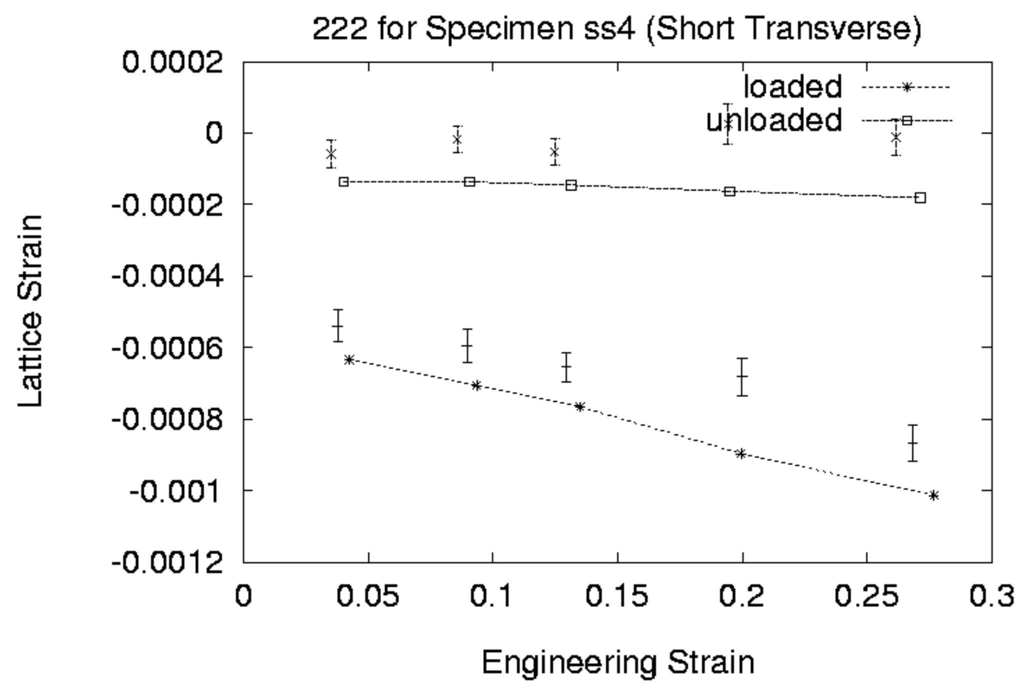
(222) Crystals

Axial Lattice Strains

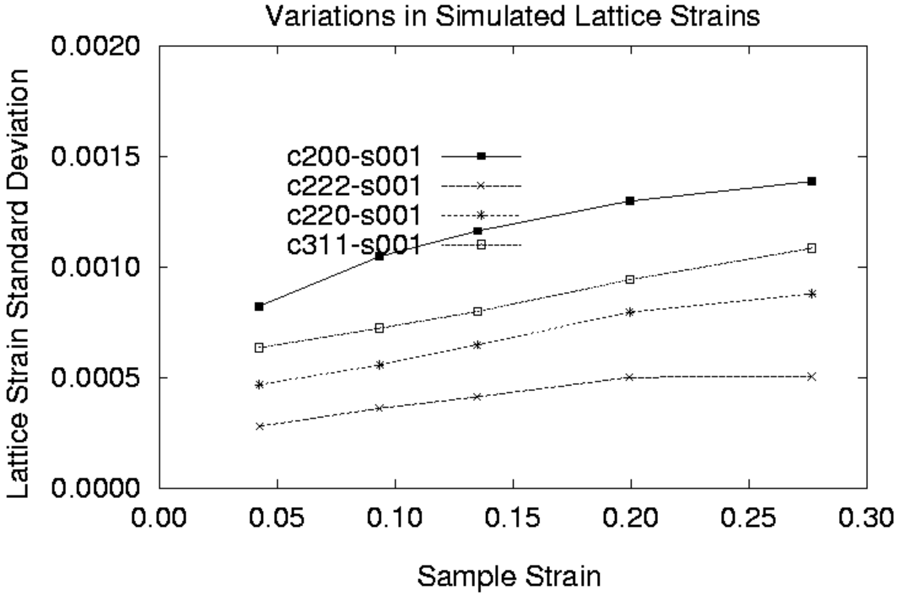
- •Upper curves - loaded
- •Lower curves - unloaded
- •Data points with error bars

Lateral Lattice Strains

- •Lower curves - loaded
- •Upper curves - unloaded
- •Data points with error bars

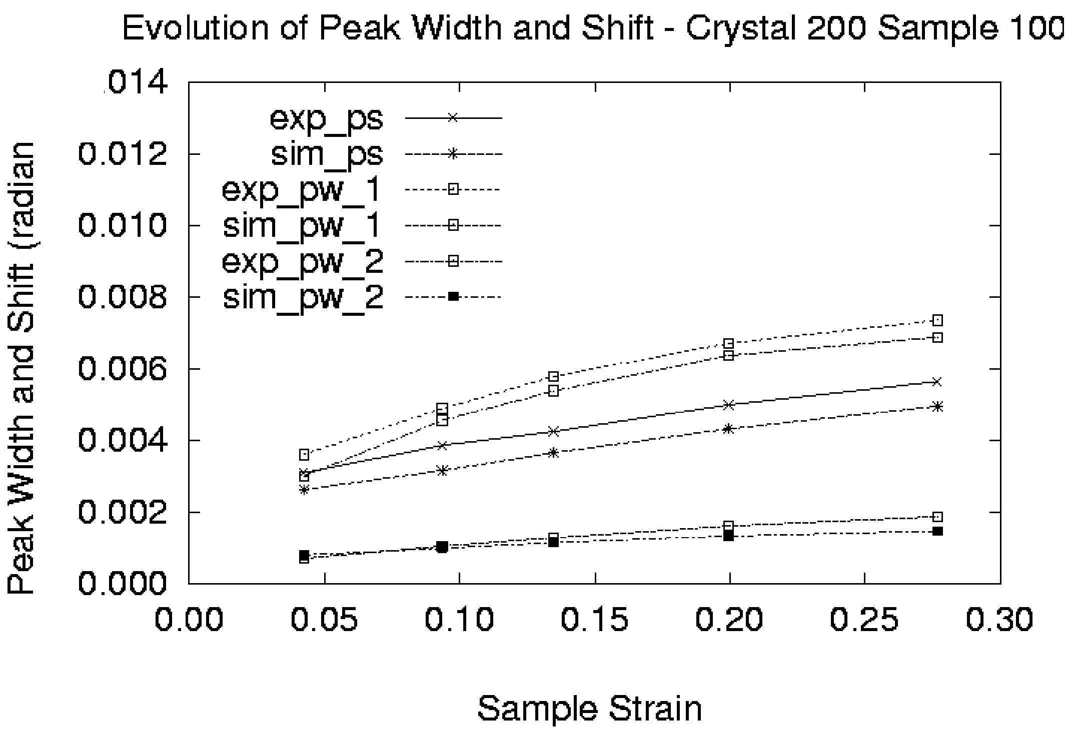


Peak Broadening - Stress Effects



Stresses:

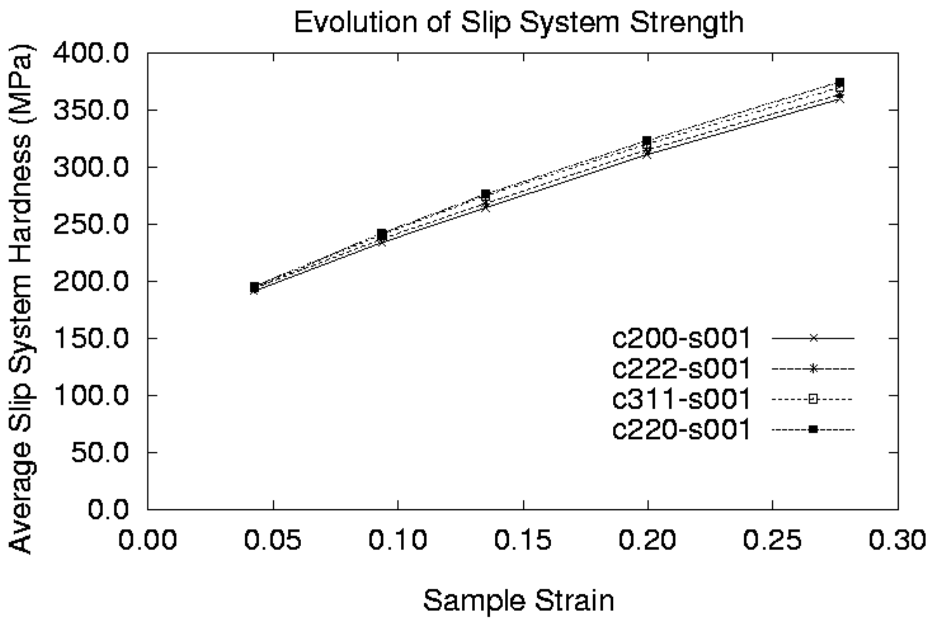
- Vary crystal to crystal
- Contribute to broadening of peaks
- Compute contribution from simulations



Peak width:

- Increases with strain
- Dislocations contribute directly and indirectly

Correlation of Increased Peak Width and Strength

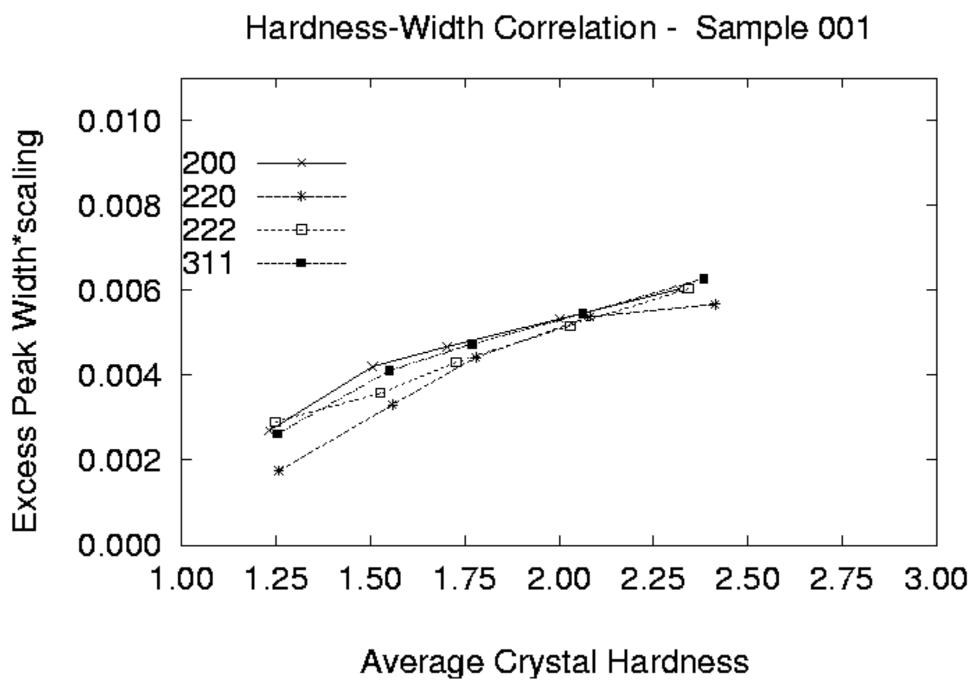


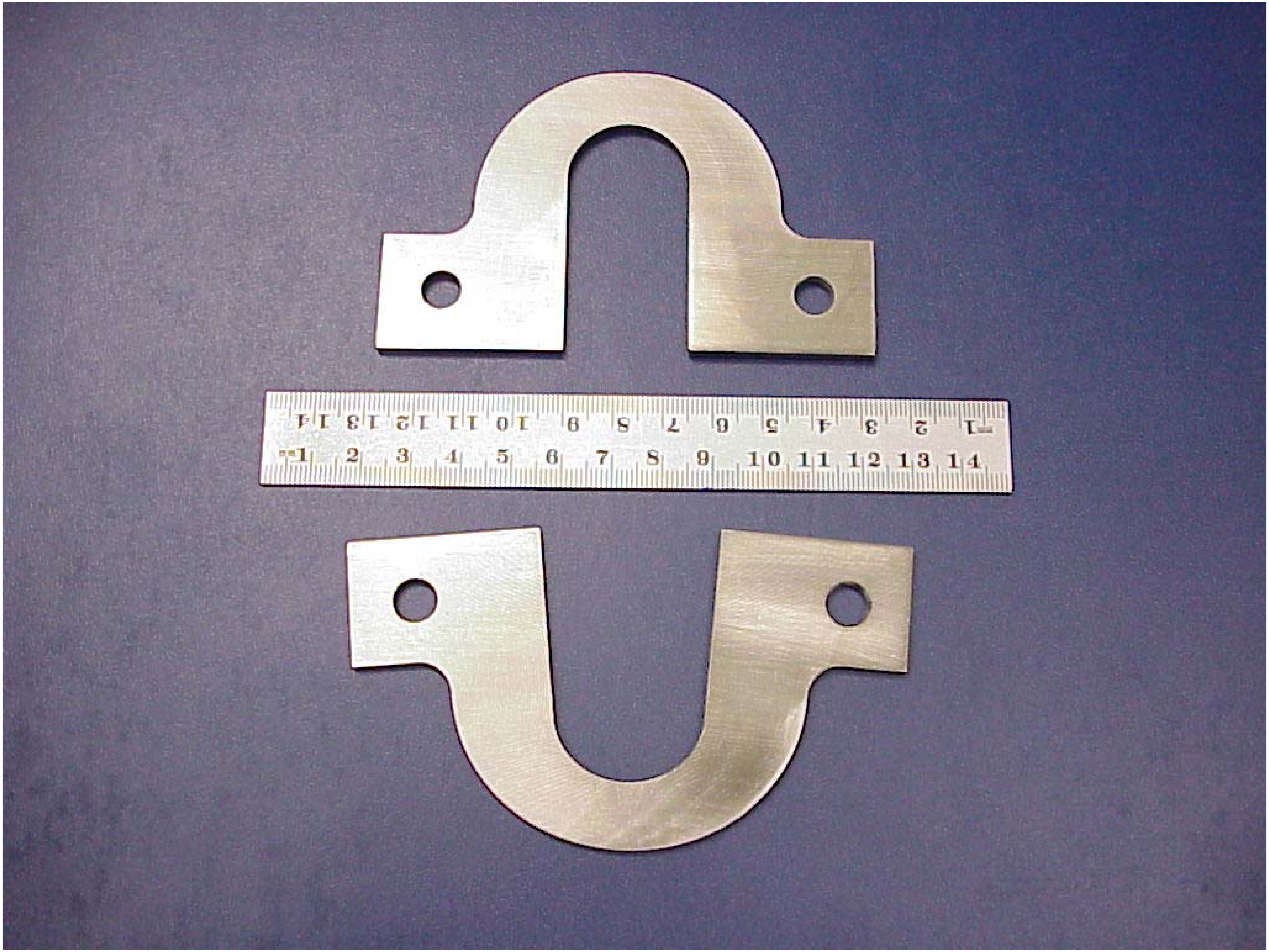
Strength:

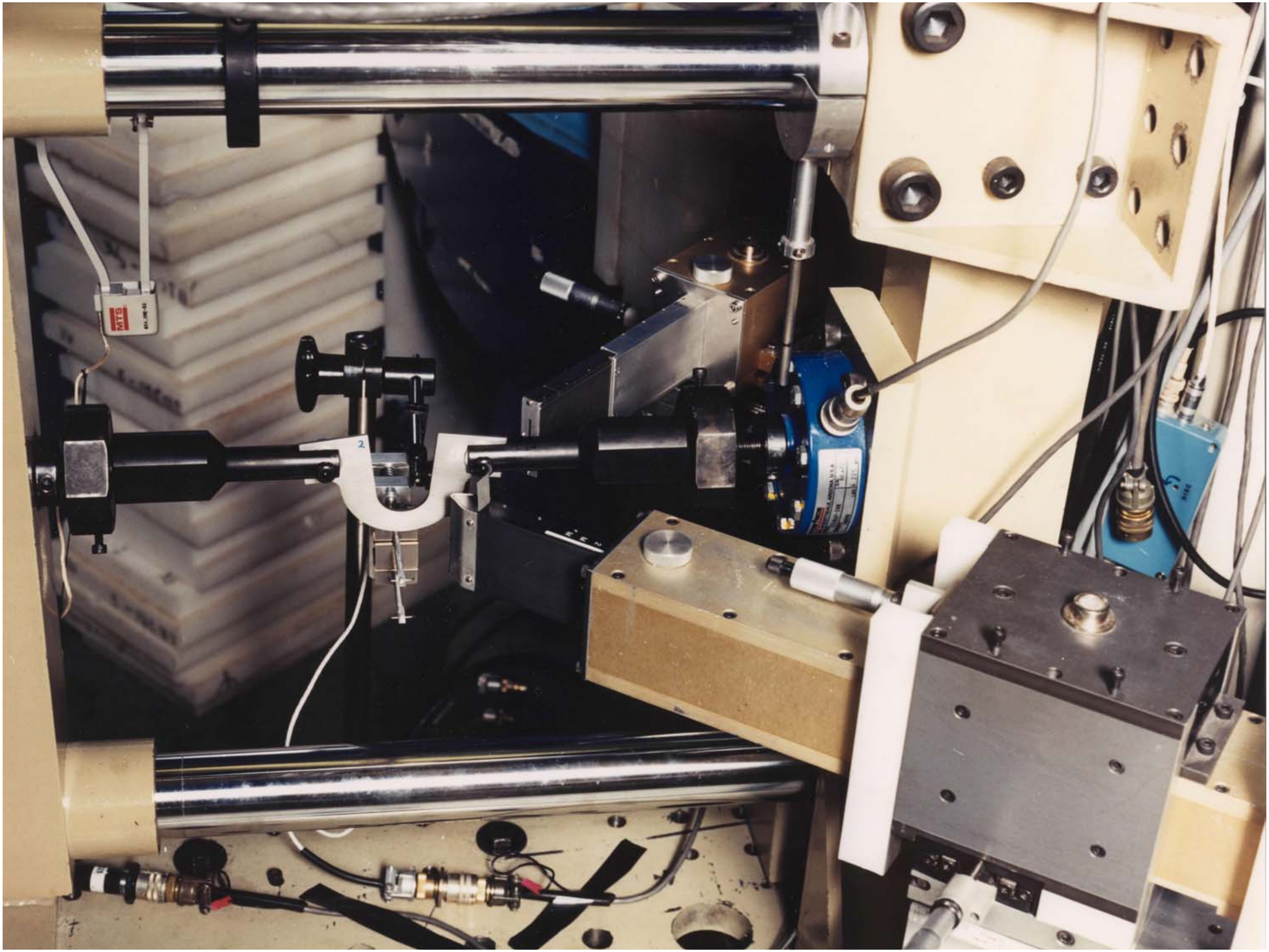
- All slip systems have equal strength
- Modified Voce hardening model
- Correlate with dislocation density

Peak broadening:

- Correlates with dislocation density
- Directly related to crystal strength



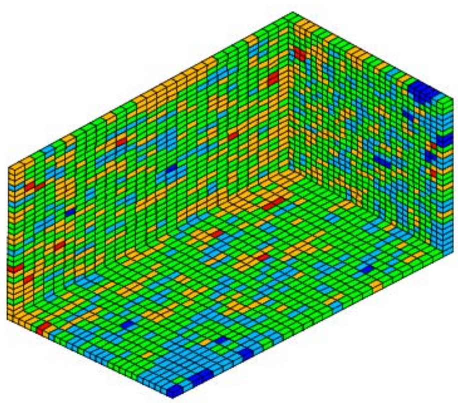

1 2 3 4 5 6 7 8 9 10 11 12 13 14



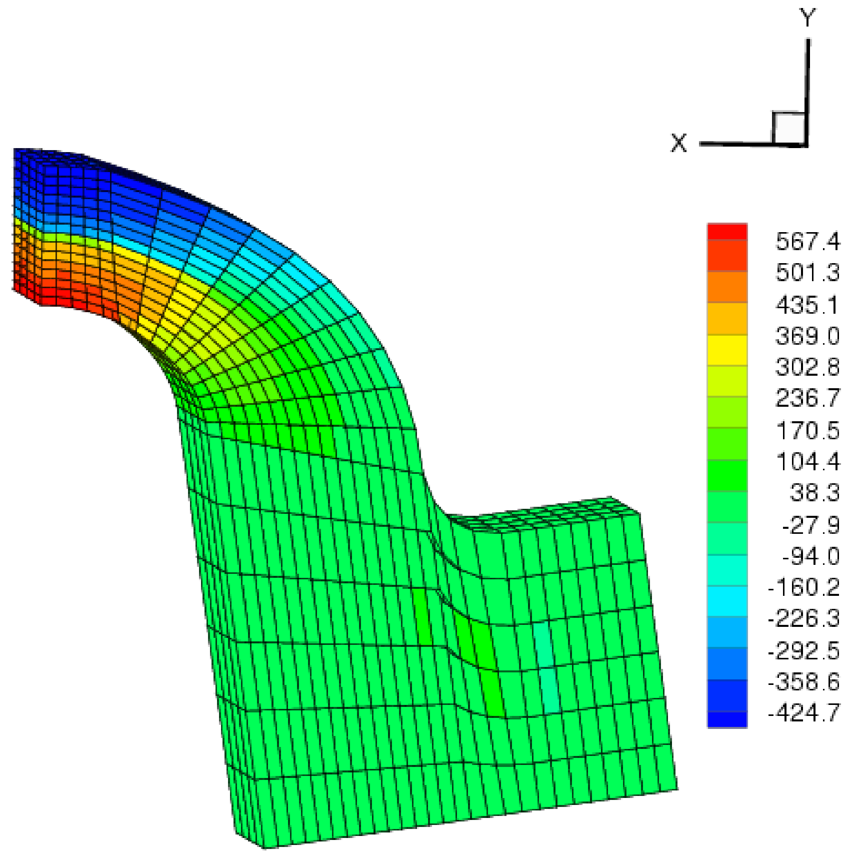
Finite Element Simulation

- Crystal-scale simulations (8 elements per crystal)
- Macro-scale simulation (crystal aggregates in every element)

Extract macro element histories and impose on diffraction volumes

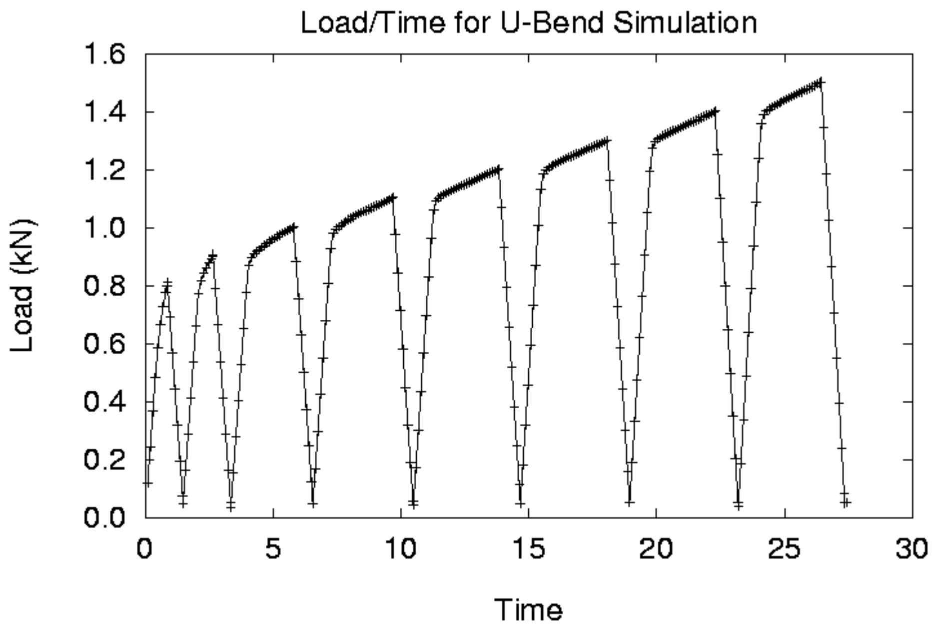


Lattice strains in polycrystal



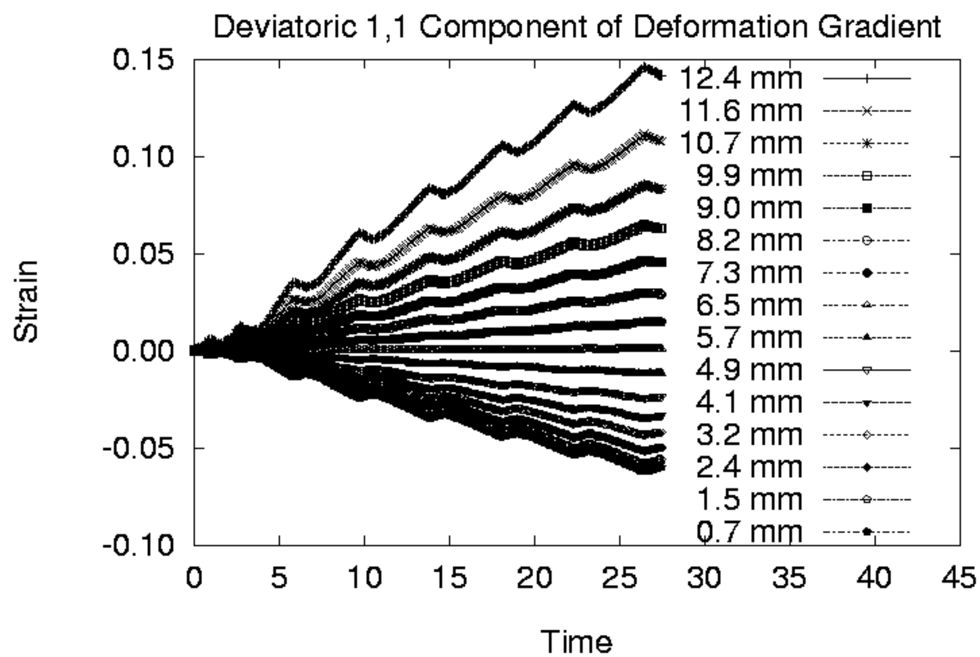
Bending stress distribution under load (MPa)

Imposed Simulation Boundary Conditions



Measured loading history
(applied to macro-scale mesh)

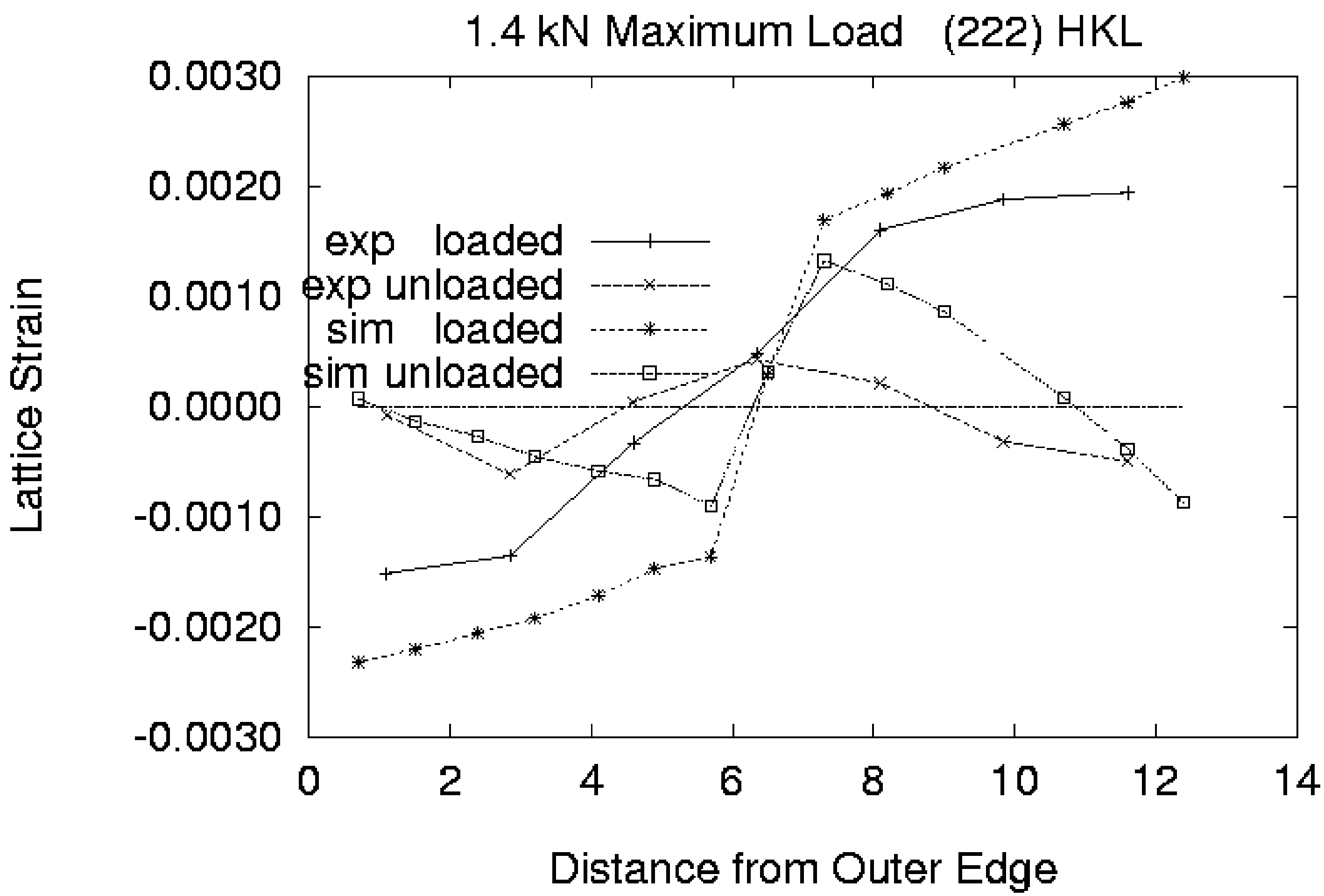
Macroscopic element histories are extracted from the macro-scale simulation and applied on the crystal-scale (diffraction volume) meshes (polycrystals)



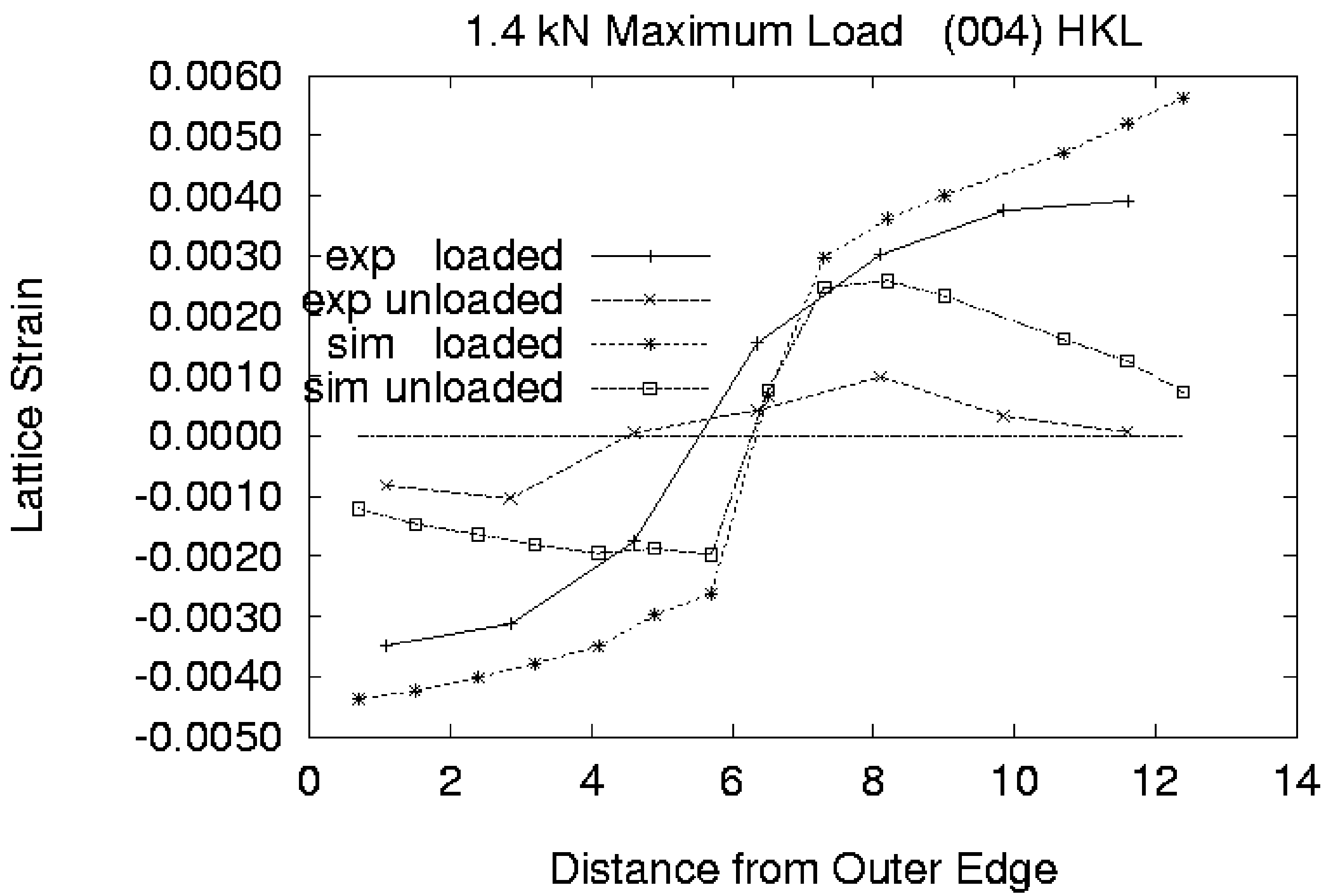
Synchronizing Macro and Crystal Scales

- Force macro and crystal scales to predict the same behavior for a tension test taken to failure
  - Slip system (plasticity) parameters determined by fitting the measured stress-strain behavior over ≈25% strain.
  - Elastic moduli (single crystal cubic) determined by:
    - Matching neutron diffraction data with crystal scale model
    - Requiring macro scale moduli to unload to zero stress over the same strain change as occurs with the crystal scale when it unloads from the same starting starting stress.
- Note:
  - Sets of single crystal elastic moduli and plasticity parameters are paired to particular modeling assumptions.
  - The set for a macro scale model differ from the set for a crystal scale model.

Lattice Strains - Measured vs Computed



Lattice Strains - Measured vs Computed



Concluding Comments

- ♦ Micromechanical models require diffraction data
  - Best means to resolve features being modeled
  - Richness of the data must be better exploited

- ♦ Coupling simulations from differing scales
  - Inadequate to determine moduli/parameters at a finer scale to be used at a coarser scale.
  - Synchronization of predictions at scale interface also is required.

- ♦ Comparisons to experiment
  - State descriptions should be based on observable features
  - Statistical measures of their distributions are essential